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Advanced modeling of large-scale oxy-fuel combustion processes

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Introduction

Oxy-fuel combustion is a promising carbon capture and storage technology and has gained increasing concerns worldwide. Combustion under oxy-fuel conditions is inherently different from conventional air-fuel combustion, among which radiative heat transfer and combustion chemistry are two of the fundamental issues. Efforts are made in both the aspects in this paper.

Methodology

Model development and verification;

Model implementation into CFD simulations of various oxy-fuel combustion processes and experimental validation.

Result

- A new weighted-sum-of-gray-gases model (WSGGM) applicable to oxy-fuel combustion derived, validated and demonstrated: extending applicability to oxy-fuel, introducing a scaling temperature for an improved WSGGM data-fitting, and covering more representative conditions to better account for the variations in H₂O/CO₂ molar ratio in oxy-fuel flames (Yin et al., 2010).
- Various combustion mechanisms implemented in CFD of oxy-fuel combustion & recommendations made in the light of experimental validation (Yin et al., 2011).

Table 1. The three global mechanisms: "WD", "WD_refined", "JL_refined".

No	Reactions	Rate equations [kmol/(m ³ ·s)]	A	b	E
WD: Westbrook & Dryer 2-step mechanism					
1	CH ₄ + 1.5O ₂ → CO + 2H ₂ O	$\frac{d[\text{CH}_4]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CH}_4]^{0.7} [\text{O}_2]^{0.8}$	5.01×10 ¹¹	0	2.0×10 ⁸
2	CO + 0.5O ₂ → CO ₂	$\frac{d[\text{CO}]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CO}] [\text{O}_2]^{0.25}$	2.24×10 ¹²	0	1.7×10 ⁸
WD_refined: refined Westbrook & Dryer 2-step mechanism for oxy-fuel combustion					
1	CH ₄ + 1.5O ₂ → CO + 2H ₂ O	$\frac{d[\text{CH}_4]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CH}_4]^{0.7} [\text{O}_2]^{0.8}$	5.03×10 ¹¹	0	2.0×10 ⁸
2	CO + 0.5O ₂ → CO ₂	$\frac{d[\text{CO}]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CO}] [\text{O}_2]^{0.25} [\text{H}_2\text{O}]^{0.5}$	2.24×10 ⁶	0	4.2×10 ⁷
3	CO ₂ → CO + 0.5O ₂	$\frac{d[\text{CO}_2]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CO}_2] [\text{H}_2\text{O}]^{0.5} [\text{O}_2]^{-0.25}$	1.10×10 ¹³	-1	3.3×10 ⁸
JL_refined: refined Jones & Lindstedt 4-step mechanism					
1	CH ₄ + 0.5O ₂ → CO + 2H ₂	$\frac{d[\text{CH}_4]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CH}_4]^{0.5} [\text{O}_2]^{1.25}$	4.4×10 ¹¹	0	1.3×10 ⁸
2	CH ₄ + H ₂ O → CO + 3H ₂	$\frac{d[\text{CH}_4]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CH}_4] [\text{H}_2\text{O}]$	3.0×10 ⁸	0	1.3×10 ⁸
3	H ₂ + 0.5O ₂ ↔ H ₂ O	$\frac{d[\text{H}_2]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{H}_2] [\text{O}_2]^{0.5}$	5.7×10 ¹¹	0	1.5×10 ⁸
4	CO + H ₂ O ↔ CO ₂ + H ₂	$\frac{d[\text{CO}]}{dt} = AT^b e^{-E/(RT)} \cdot [\text{CO}] [\text{H}_2\text{O}]$	2.8×10 ⁹	0	8.4×10 ⁷

- Non-gray vs. Gray calculation of the Yin et al. (2010) oxy-fuel WSGGM vs. Gray calculation of the Smith et al. (1982) WSGGM in oxy-fuel combustion (Yin, 2012).

Conclusions

- The original WD 2-step over-predicts flame temperature & largely under-predicts CO level;
- The refined WD 2-step & JL 4-step reasonably predict the high CO level in oxy-fuel. The refined JL 4-step also reasonably predicts H₂ & flame temperature;
- Applied to small-scale oxy-fuel combustion modeling ($L < a$ few meters), different WSGGMs make negligible difference.

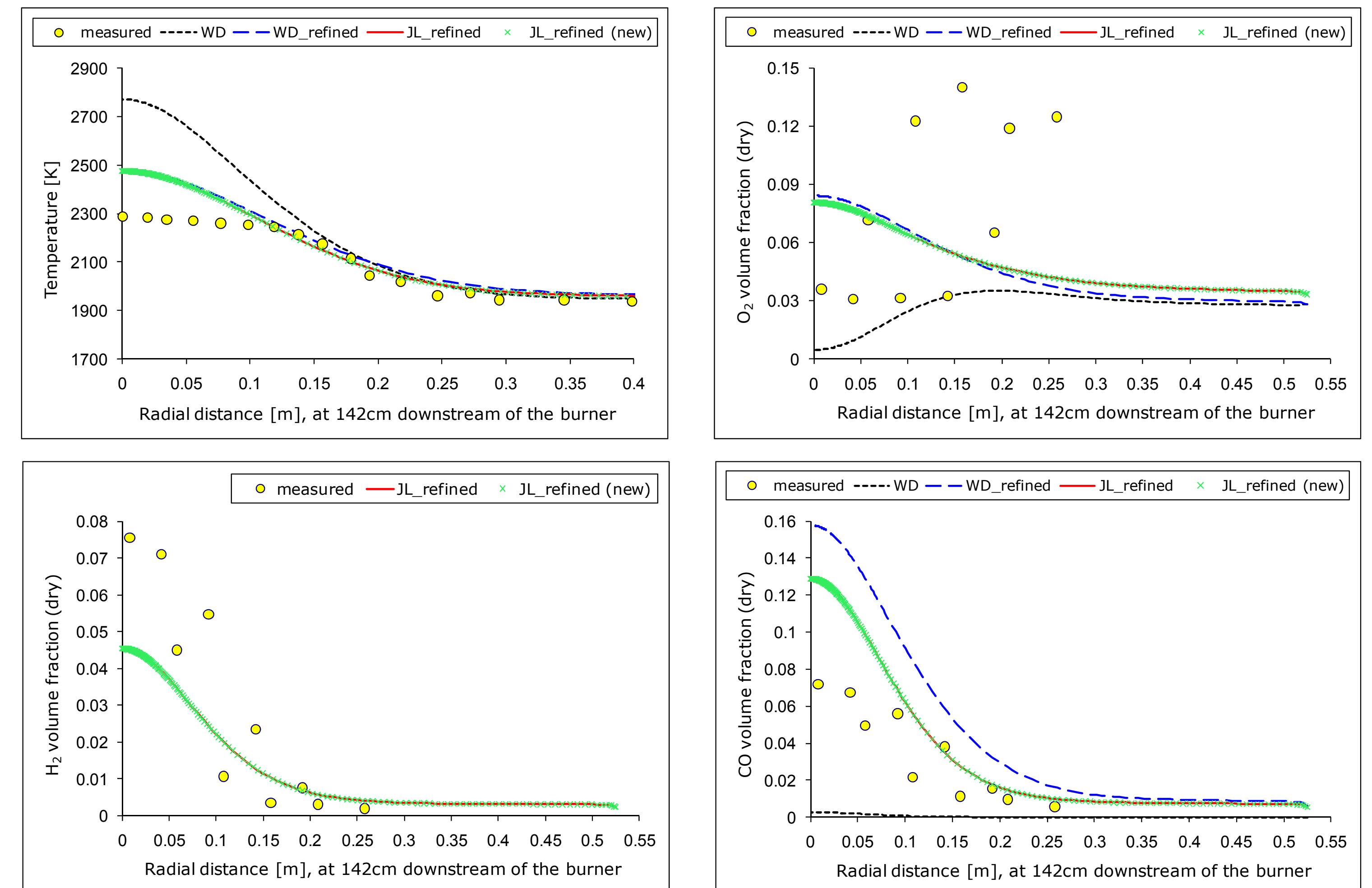


Figure 1. CFD of IFRF 0.8MW oxy-NG furnace, using different mechanisms & gaseous radiative property models [Smith et al. (1982) WSGGM by default, Yin et al. (2010) WSGGM as "new"; both gray calculations].

Case	Model for radiative properties	Sub-models in common
Case-0	The Smith et al. (1982) WSGGM, gray cal.	Fine structured mesh, standard k-ε, DO (2×2×8 directions), refined WD 2-step / EDC.
Case-1	The Yin et al. (2010) WSGGM, gray calculation	
Case-2	The Yin et al. (2010) WSGGM, non-gray cal.	

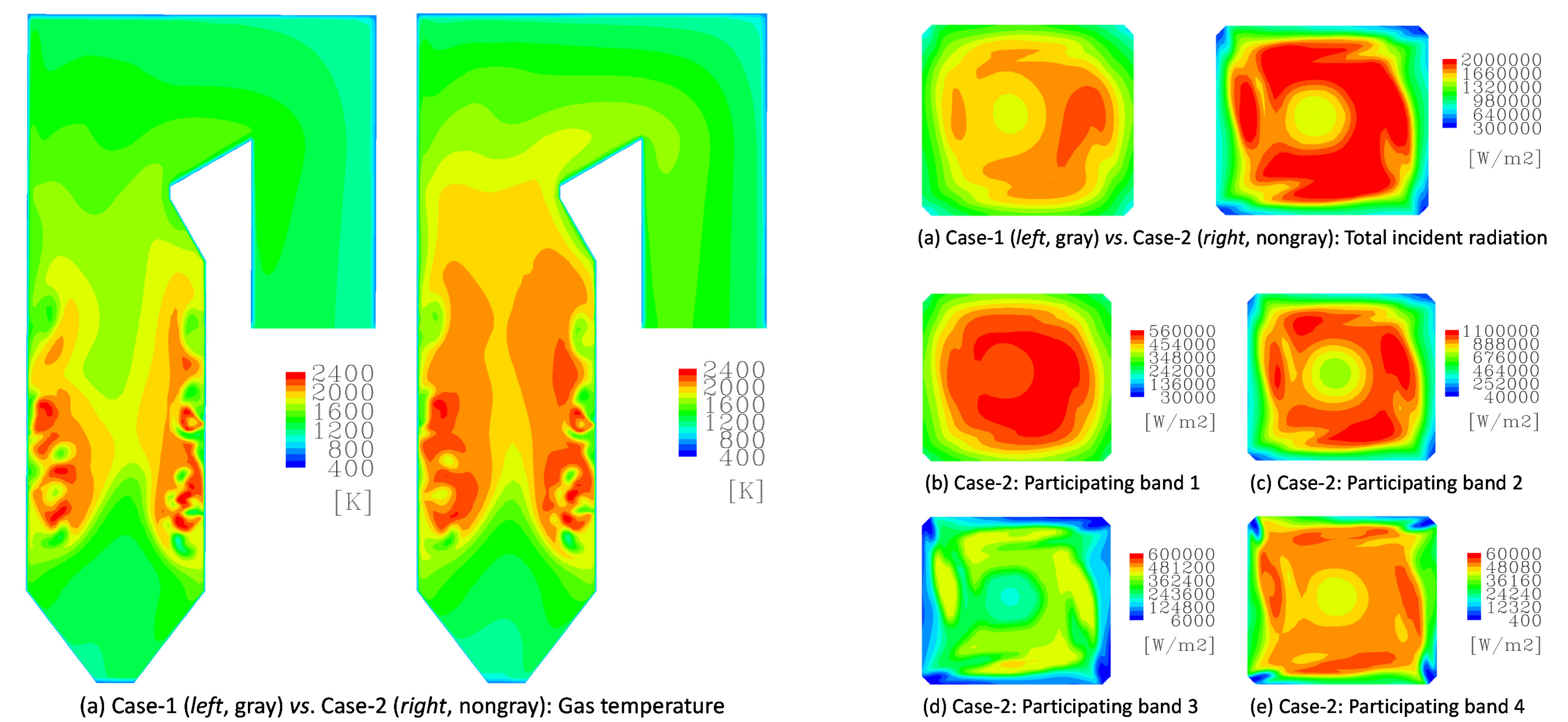


Figure 2. CFD results of a 1500MW (thermal input) utility boiler assumed to be operating under oxy-fuel condition with dry flue gas recycle.

- Gray/non-gray of the same WSGGM make distinct difference, more remarkable than that between gray calculation of different WSGGMs;
- Gray calculation over-predicts radiative HT to furnace walls, under-predicts gas temperature in furnace, and results in a higher CO prediction;
- The demonstrated nongray-gas effects also apply for air-fuel conditions; may be compromised in solid-fuel combustion.

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